Structure and magnetization of a two-dimensional vortex liquid in the presence of strong pinning

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The structure of a two-dimensional vortex liquid in the presence of strong pinning centers is investigated using the density-functional formalism. Short-range positional and angular correlations in the liquid result in an effective interaction between pinned vortices, mediated by the unpinned ones. This effective interaction is short range and it oscillates with the intervortex distance. Matching of this oscillation with a periodic array of strong pinning centers leads to anomalies in the reversible magnetization $M(H)$ at the ''matching field'' B_ϕ and some of its harmonics. [S0163-1829(98)02714-3]

I. INTRODUCTION

The existence of a vortex liquid phase is one of the key features of high-temperature superconductors in the mixed state. Thermal fluctuations are responsible for melting the Abrikosov vortex lattice at $B_m(T)$, well below the (mean-field) critical field $B_{c2}(T)$.[1] This gives rise to a phase lacking long-range order, but where fluctuations are believed to be structured into thermally wandering vortex lines forming a line liquid. Depending on the magnetic field and the temperature, the vortex lines may break up into weakly coupled stacks of two-dimensional ''pancake'' vortices lying on the superconducting layers. In the presence of quenched disorder produced by randomly placed pinning defects, the vortex lattice lacks long-range translational order, but remains pinned at low currents, with an irreversible magnetization. In the case of weak disorder, this is essentially due to a nonvanishing shear stiffness. On the other hand, since the vortex liquid cannot sustain shear and therefore cannot be pinned by weak disorder, it displays reversible properties. Thus, the presence of quenched disorder leads to an irreversibility line which, in general, is different from the melting line of the pure system. Fluctuations induced in the lattice by weak impurity disorder add to the thermal fluctuations and lower the melting field, thus extending the liquid phase domain.[2] In contrast, strong and correlated quenched disorder such as that produced by irradiation-induced columnar defects have a confining effect on the thermal wandering of vortex lines and can push the melting (or irreversibility) line upwards, thus reducing the liquid phase domain. This occurs for defect densities larger than the vortex density, i.e., for B smaller than the ''matching field'' B_ϕ, defined as $B_\phi \equiv \Phi_0 n_d$ where $\Phi_0 = hc/2e$ is the flux quantum, and n_d is the number of columnar defects per unit area. However, a liquid phase is expected[3] to be present at sufficiently high temperatures if $B > B_\phi$. The basic thermodynamic properties of such a liquid are expected to be strongly modified due to the presence of the strong pins. This has been demonstrated by the experimental evidence[4–6] of anomalies in the reversible magnetization curve $M(H)$ near B_ϕ in irradiated Tl- and Bi-based cuprate crystals. For higher fields, no anomalies have been detected so far, probably due to the random character of the pin array. On the other hand, for artificial periodic pin arrays, anomalies have been found[7] in the irreversible (vortex solid) regime at harmonics of the matching field. Also, Lorentz microscopy imaging[8] of vortices in the presence of periodic pin arrays have revealed interesting commensurate structures.

In this paper, we show that long-range correlations in the positions of the vortices are not essential for such phenomena, and that similar effects also occur in the liquid phase, due to short-range correlations present in the liquid. For this problem, due to the specific properties of the liquid state, such as short-range translational correlations and enhanced thermal fluctuations, it is clear that one cannot rely on the usual vortex-lattice free energy. This work reports the first direct calculation of the properties of a vortex liquid in the presence of strong disorder. For this purpose we use the density-functional (DF) formalism,[9] which allows us to take into account the competition between entropic[10] and interaction effects in the liquid state. For the sake of simplicity, we consider a purely two-dimensional (2D) vortex liquid. This is a reasonable approximation in a large part of the (B,T) phase diagram of extremely anisotropic layered superconductors such as $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) in a magnetic field perpendicular to the layers, especially in high fields where the two-dimensional layers of ''pancake'' vortices are decoupled.[11] More generally, our calculation may apply to the case of a thin film for which the ''confinement length'' by columnar defects exceeds the film thickness. As discussed later, it would be quite straightforward to extend our calculations to a layered superconductor in which both the external magnetic field and the straight columnar defects are perpendicular to the layers. The formalism developed in this paper would also be applicable to other 2D systems (such as magnetic bubble arrays[12] and charge-density-wave systems[13]) in the presence of strong pinning disorder.

Let us summarize the main results of this work. First, given a single defect that pins a vortex, we calculate the azimuthally symmetric liquid density in the vicinity of the defect, showing that it is inhomogeneous and oscillating, the

liquid density being depleted in the vicinity of the pinned vortex. This effect disappears with increasing temperature as the vortex becomes thermally depinned. Then, given two pinned vortices, we obtain an oscillatory effective interaction as a function of their separation. Due to the breaking of rotational symmetry in this case, angular correlations also appear but never happen to be large. We qualitatively compare the found behavior with decoration experiments,[14–16] in which the field-cooled liquid is believed to freeze close to the irreversibility line, thereby representing in some sense a snapshot of the liquid close to freezing. As another application, we calculate the magnetization in the presence of a square pin array and find anomalies in the reversible magnetization at the matching field and at some of its harmonics. This points towards another motivation of this work: if periodic pin arrays can be fabricated in high-T_c materials, then measurements of the magnetization in the liquid state can give, through the present work, access to fundamental liquid-state quantities such as correlation functions of the density. This is important because extraction of such information by other means (e.g., from neutron-scattering measurements) appears to be very difficult.

We describe the model and the formalism in Sec. II. Section III is concerned with our single and two-pin calculations. Section IV describes the calculations for a periodic array of pins. We end with conclusions and discussions.

II. MODEL AND FORMALISM

The DF formalism is one of the major tools in studies of classical liquids.[17] It has also been recently applied to vortex matter, to determine the freezing (melting) line in a clean layered superconductor[18,19] and also in the presence of weak pinning disorder.[2] In this paper, we extend the DF approach to strong disorder, considering for simplicity a purely 2D vortex liquid and examining its spatial density fluctuations in the presence of strong attractive pinning centers. We shall hereafter consider (unless otherwise stated) the case $B>B_\phi$ and temperatures well below the thermal depinning temperature, so that nearly all defects pin a vortex.

In the London approximation, point vortices in a single superconducting layer have logarithmic interactions, $\beta V(r) = -\Gamma \ln(r/\xi)$, where $\Gamma=\beta\Phi_0^2 d/(8\pi^2\lambda^2)$. Here $\beta=1/(k_B T)$, d the effective layer thickness (typically one unit cell for layered superconductors), ξ the Ginzburg-Landau coherence length and λ the London screening length in the layers. Defining a length a_0, related to the homogeneous vortex liquid density $\rho_l \equiv B/\Phi_0$ by $\pi a_0^2 \rho_l = 1$, the nearest and next-nearest neighbor distances in the triangular lattice are $1.9a_0$ and $3.3a_0$, respectively. For parameter values appropriate for BSCCO [$\lambda(T=0)=1500$ Å, $d=15$ Å, $T_c(H=0)=90$ K], the dimensionless coupling constant Γ is approximately $\Gamma \approx 2.4\times 10^3/(T \text{ in kelvin})$ at low temperatures where the dependence of λ on the temperature can be neglected.

A defect (pinning center) at the origin is assumed to produce a potential of the form $V_p(r) = -V_0(1-r^2/a^2)$ if $r \leq a$, and $V_p(r)=0$ if $r>a$. The potential strength is $\beta V_0 \approx \Gamma/4\{0.5+\ln[1+(a^2/\xi^2)]\}$.[1] We hereafter choose $\beta V_0 = \Gamma/4$ and $a=0.1a_0$ when unspecified. For columnar pins with $a\approx 5$ nm, this amounts to $B\approx 0.25$ T. One should note that contributions to the pinning of a given vortex also come from defects that do not contain its core. This is due to the perturbation of the screening currents by the insulating regions associated with such defects. However, in high fields, these contributions are screened[20] and only add some weak pinning. Such contributions are neglected here. We also assume that a pinning center does not pin more than one vortex.

In the absence of pins, the homogeneous vortex liquid is characterized by its direct (Ornstein-Zernike) pair-correlation function[17] $c(\mathbf{r},\mathbf{r}')=c(|\mathbf{r}-\mathbf{r}'|)$, which represents the coupling between density fluctuations at points $\mathbf{r}$ and $\mathbf{r}'$. The values of $c(r)$ used here are taken from a calculation[19] based on an approximation proposed by Rogers and Young.[21] From comparisons with simulation data, it is known[19] that this approximation is fairly accurate, but it slightly underestimates the correlations in the liquid at temperatures close to its equilibrium crystallization temperature. We do not attempt to derive a self-consistent form for $c(r)$ in the presence of the random pinning potential. This is surely reasonable in the case of a dilute defect array. Moreover, even close to the matching field, where vortex fluctuations are severely quenched by pinning, this hypothesis is comparable to a similar assumption that is commonly made in DF calculations of crystallization transitions[9] where one uses the correlation function of the homogeneous liquid to calculate the free energy of the ordered solid.

The DF formalism involves the use of an expression for the free energy F of an inhomogeneous state, characterized by the density distribution $\rho(\mathbf{r})$, as a functional of $\rho(\mathbf{r})$. In this work, we use a density functional of the form proposed by Ramakrishnan and Yussouff:[9]

$$\beta(F-F_l)=\int d\mathbf{r}\left(\rho(\mathbf{r})\ln\frac{\rho(\mathbf{r})}{\rho_l}-\delta\rho(\mathbf{r})\right)+\beta\int d\mathbf{r}\,v(\mathbf{r})\,\delta\rho(\mathbf{r}) - \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\,c(|\mathbf{r}-\mathbf{r}'|)\,\delta\rho(\mathbf{r})\,\delta\rho(\mathbf{r}'), \qquad (1)$$

where $\delta\rho(\mathbf{r})\equiv\rho(\mathbf{r})-\rho_l$, F_l is the free energy of the uniform liquid of density ρ_l and $v(\mathbf{r})$ is the external one-body potential (here the pinning potential).

The vortex liquid is homogeneous [i.e., $\rho(\mathbf{r})=\rho_l$ for all $\mathbf{r}$] in the absence of pinning. The presence of pinning centers causes the time-averaged local density to be inhomogeneous even in the liquid state. Our strategy is to characterize this inhomogeneity by appropriate variational forms involving a few variational parameters, and to determine the values of these variational parameters by minimizing the free energy given by the expression of Eq. (1). The details of the calculations and the results are described in the next two sections.

III. SINGLE AND TWO-PIN CALCULATIONS

Let us first consider a 2D vortex liquid in the presence of a single strong pinning center at the origin that traps one vortex. This obviously breaks translational symmetry, thereby making the average density $\rho(\mathbf{r})$ in the neighborhood of the pinning center *inhomogeneous*, with azimuthal symmetry. The pinned vortex gives rise to a sharp peak in $\rho(\mathbf{r})$, which is centered at the origin and whose width is expected to be approximately equal to the range a of the pinning potential. The integrated weight under this peak is

expected to be close to unity if one vortex is trapped at the pinning center. For a perfect pin (δ-function potential), the function $\rho(r)$ for $r \neq 0$ is, according to the Percus theorem,[17] identical to the pair distribution function $g(r)$ of the homogeneous liquid that describes the short-range positional correlations present. In particular, the liquid density is expected to be depleted in the immediate vicinity of the pinned vortex. Beyond this ''correlation hole,'' a damped density wave with a period close to the nearest-neighbor spacing ($\approx 1.9a_0$) of a triangular lattice of density ρ_l should appear. The case of a strong pin with a finite pinning potential that has a short but nonzero range should be qualitatively similar. We therefore choose a simple variational ansatz for the average density near the pinning center:

$$\rho(r) = \rho_l + \rho'(r); \quad \rho'(r) \equiv a_1 e^{-b_1 r^2} + f(r),$$

$$f(r) = a_2 J_0(G r_m) \quad \text{for} \quad r \leq r_m,$$

$$f(r) = a_2 e^{-b_2 (r - r_m)} J_0(G r) \quad \text{for} \quad r > r_m. \qquad (2)$$

Here, the first term in $\rho'(r)$ represents the part of the total density that arises from the vortex pinned at the defect. It displays a Gaussian broadening due to the finite strength and nonzero range of the pinning potential. The second term, $f(r)$, describes the correlation hole and the oscillatory density modulation in the vicinity of the pinning center. It involves an integration of a lattice density wave $e^{i\mathbf{G}\cdot\mathbf{r}}$ over the polar angle, $\mathbf{G}$ being one of the shortest reciprocal lattice vectors of a triangular lattice of density ρ_l. The cutoff r_m denotes the first minimum of the Bessel function $J_0(Gr)$. This form is by construction close to the homogeneous liquid pair distribution function $g(r)$. It is, therefore, physically sound and we have found that it yields the lowest free energy among other similar choices. The variational parameters a_1 and b_1 describe, respectively, the *strength* and the *range* of the pinning at the origin, while a_2 and b_2 describe, respectively, the *amplitude* and the *range* of the density modulation near the pinned vortex.

Using Eqs. (1) and (2), we have carried out a numerical minimization of the excess free energy induced by a single pin as a function of the four parameters a_1, b_1, a_2, and b_2. The minimization is done under the following constraints: (i) the density at every point must remain non-negative; (ii) the integral of ρ', the deviation of the local density from the average value, must be equal to zero (conservation of the number of vortices). Since both the functions appearing in the expression for ρ' are short-range, nonzero contributions to the integrals of Eq. (1) come only from regions close to the origin, and it is not difficult to evaluate these integrals numerically [the double integral appearing in the third term of Eq. (1) is evaluated by converting it into a single integral in Fourier space]. We have carried out this calculation for a number of values of Γ in the range $50 \leq \Gamma \leq 120$, which corresponds to temperatures in the range between 45 and 20 K for BSCCO. We note that these temperatures are higher than the equilibrium crystallization temperature of the vortex system without disorder, which is estimated from molecular-dynamics simulations[22] to correspond to $\Gamma \simeq 140$. If we keep the value of βV_0 fixed at $\Gamma/4$ (see Sec. II), then we find that the optimal values of the variational parameters a_1 and b_1 are such that the integrated weight of the Gaussian term appearing in the expression for $\rho'(r)$ [Eq. (2)] remains very close to unity for all values of Γ, indicating that the pinning center traps one vortex at all temperatures lying in the range considered. These temperatures are, therefore, lower than the so-called thermal depinning temperature $T_{\rm dp}$. The optimal value of b_1 is found to be quite close to the expected value, $\beta V_0 / a^2$, where a is the range of the parabolic pinning potential. Figure 1 shows a plot of the radial density profile $f(r)$ outside the range of the pinning potential as a function of the distance r at a temperature corresponding to $\Gamma = 50$. We also show on the same plot the pair distribution function $g(r)$ of the homogeneous liquid, calculated from the data for $c(r)$ used in the evaluation of the free energy. As expected, $f(r)/\rho_l$ is very similar to $g(r)$, with slightly less-pronounced oscillations due to imperfect localization of the vortex at the origin. These results indicate that the variational ansatz of Eq. (2), together with the Ramakrishnan-Yussouff free-energy functional of Eq. (1), provide a good description of the density inhomogeneity produced in the vortex liquid by a single strong pinning center.

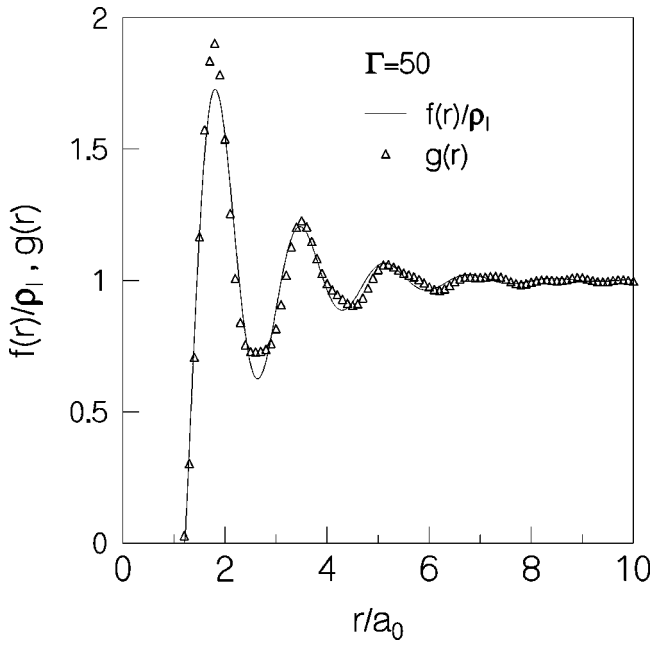

FIG. 1. The optimal density profile $f(r)$ near a pinning center [see Eq. (2)], normalized by the average density ρ_l, and the pair distribution function $g(r)$ for $\Gamma = 50$. The distance r is measured in units of a_0 defined by $\pi a_0^2 \rho_l = 1$. The curve for $f(r)/\rho_l$ has been shifted upward by one unit in order to bring out its similarity with $g(r)$.

To study the process of thermal depinning of vortices from the defects, we repeated the calculation described above for a number of different values of βV_0 and Γ, treating them as independent parameters. The optimal values of the variational parameters a_1, b_1, c_1, and d_1 were determined for each pair of values of βV_0 and Γ. The probability of the pinning defect being occupied by a vortex was then obtained as the integral of the Gaussian term in the expression for the density [Eq. (2)]. The results for this occupation probability as a function of βV_0 for three different values of Γ are shown in Fig. 2. It is clear from the data that the occupation probability is very close to unity (i.e., the vortex

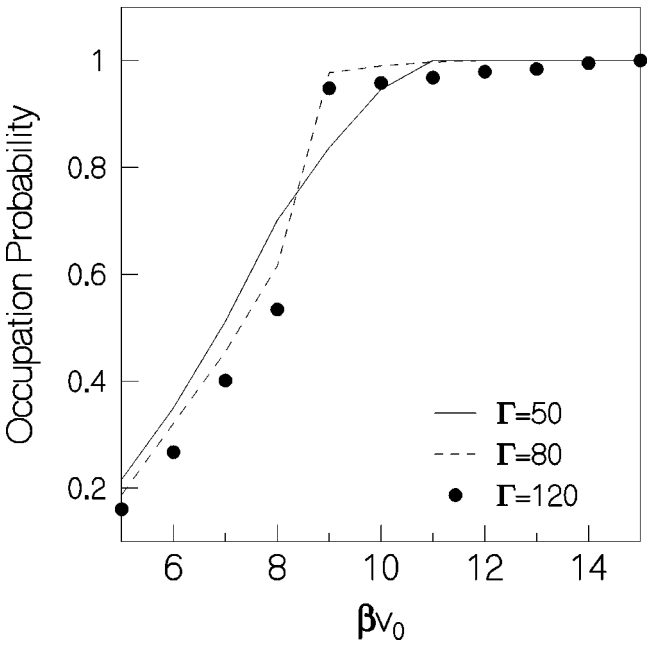

FIG. 2. The probability of occupation of a pinning center as a function of βV_0 where V_0 is the depth of the pinning potential and β is the inverse temperature. The data for three values of the dimensionless coupling constant Γ (see text) are shown.

is fully pinned at the defect) for $\beta V_0 > 8$, and that it begins to decrease below unity (i.e., the vortex begins to get thermally depinned) as βV_0 is decreased below $\beta V_c \simeq 8$. The decrease of the occupation probability as βV_0 is decreased below βV_c becomes sharper as the value of Γ is increased (i.e., as the temperature is decreased). However, the value of βV_c appears to be nearly independent of the value of Γ in the range considered. Using parameter values appropriate for BSCCO and the two-fluid form for the temperature dependence of λ, we find that $\beta V_0 \approx 8$ corresponds to a temperature of about 60 K. Since the occupation probability decreases smoothly to zero as βV_0 is decreased below βV_c, it is difficult to identify a particular temperature as the depinning temperature $T_{\rm dp}$. Our results, however, predict that nearly all vortices will be thermally depinned at temperatures corresponding to $\beta V_0 \leqslant 4$.

Let us now consider two defects with spacing d, each of them pinning a vortex, thus generating an oscillating density wave in its vicinity. The matching of these density waves leads to commensurability effects between the interdefect distance d and the length a_0. These effects come from two-body correlations which, in two dimensions, introduce not only radial but also angular short-range correlations, reflecting a tendency of vortices surrounding a pinned one to organize into predominantly hexagonal arrangements without a fixed orientation. When two pinned vortices are nearby, one expects an interaction that tries to lock together the local orientations around the two pinned vortices. The range of this interaction is expected to be roughly that of $g(r)$ but its detailed form is unknown. In order to evaluate it, we write the density distribution in the neighborhood of two pinning centers located at $\mathbf{R}_1$ and $\mathbf{R}_2$ as a simple superposition of individual density waves:

$$\rho(\mathbf{r}) = \rho_l + a_1 e^{-b_1 r_1^2} + a_1 e^{-b_1 r_2^2} + f'(\mathbf{r}_1) + f'(\mathbf{r}_2), \quad (3)$$

where $\mathbf{r}_i \equiv \mathbf{r} - \mathbf{R}_i$, $i = 1,2$, and the new function f' includes the possibility of a sixfold angular modulation of the density,

$$f'(\mathbf{r}_i) = a_2 J_0(G r_m) \quad \text{for} \quad r_i \leqslant r_m,$$

$$f'(\mathbf{r}_i) = a_2 e^{-b_2(r_i - r_m)} \Bigg[(1-\alpha) J_0(G r_i) + \alpha \frac{1}{6} \sum_{k=1}^{6} e^{i \mathbf{G}_k^i \cdot \mathbf{r}_i} \Bigg] \quad \text{for} \quad r_i > r_m. \quad (4)$$

Here the quantity α, $0 \leqslant \alpha \leqslant 1$, describes the amount of rotational symmetry breaking in the density wave near each pinned vortex, which is introduced by means of the second term in the bracket in Eq. (4). The vectors $\{\mathbf{G}_k^i\}$, $k = 1,2,\ldots,6$ represent the six shortest reciprocal lattice vectors of a triangular lattice of density ρ_l. The two sets of vectors $\{\mathbf{G}_k^1\}$ and $\{\mathbf{G}_k^2\}$ at the two pinning centers make angles θ_1 and θ_2 (modulo 60°) with the line joining the pinning centers.

We first describe the results of a calculation in which the parameter α is set equal to zero, i.e., the possibility of angular modulation of the density near the pinning centers is not taken into account. For each value of the separation $d \equiv |\mathbf{R}_1 - \mathbf{R}_2|$, the free energy obtained by using the expression of Eq. (3) for the density in Eq. (1) is numerically minimized with respect to the four variational parameters a_1, b_1, c_1 and d_1. This minimization is carried out under the two constraints mentioned above and an additional one that ensures the existence of a ''correlation hole'' outside each of the two pinning centers. Operationally, the third constraint amounts to ensuring that the density vanishes immediately outside the range of the pinning potential of each pinning center. For $d \geqslant a_0$, we find that the optimal values of a_1 and b_1 correspond to full occupation of the two pinning centers. Typical results for the dependence of the free energy of a pair of pinned vortices on the separation d are shown in Fig. 3. As expected, commensurability oscillations occur as a function of the intervortex separation d: the free energy exhibits local minima at values of d corresponding to the first two maxima of $f(r)$ (see Fig. 1), and the minima of $f(r)$ correspond to local maxima of the free energy as a function of d. However, the energy scale associated with these oscillations is rather small compared to the pinning energy. It is, therefore, not surprising that the ''frustration'' caused by incommensurability is not sufficient to prevent simultaneous occupation of two pinning sites separated by a distance $d \geqslant a_0$. This is consistent with decoration experiments,[14] which show that almost every pinning site is occupied by a vortex when the number of pinning sites is smaller than the number of vortices. The occupation probability of the pinning centers begins to decrease below unity as the value of d is decreased below a_0, indicating that two pinning centers separated by distances much smaller than a_0 are not likely to be occupied simultaneously. It would be interesting to look for this effect by examining closely the images obtained from decorations experiments[14] in which the positions of both the pinning defects and the vortices are determined simultaneously.

We now consider the possibility of a nonzero angular modulation ($\alpha \neq 0$). In the first calculation we carried out to examine this possibility, the values of the variational param-

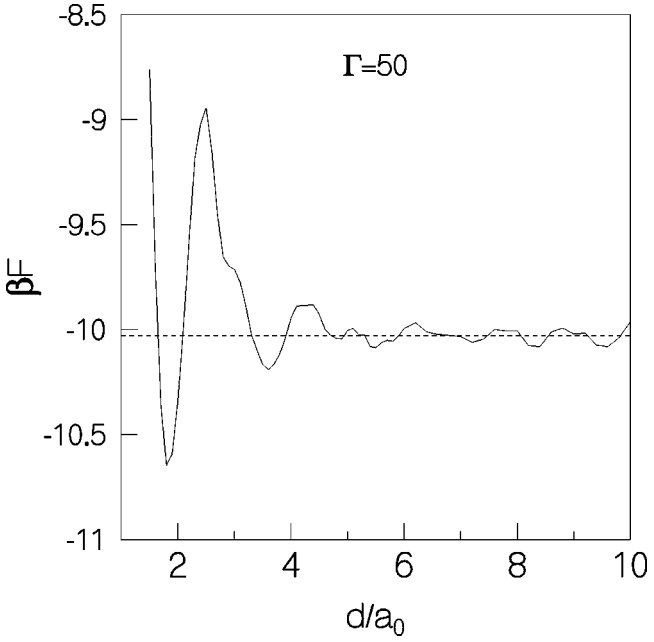

FIG. 3. The pinning contribution to the free energy of a pair of vortices trapped at two defects separated by distance d. The dotted line represents the value of βF as $d \to \infty$, obtained as two times the free energy of a single pinned vortex.

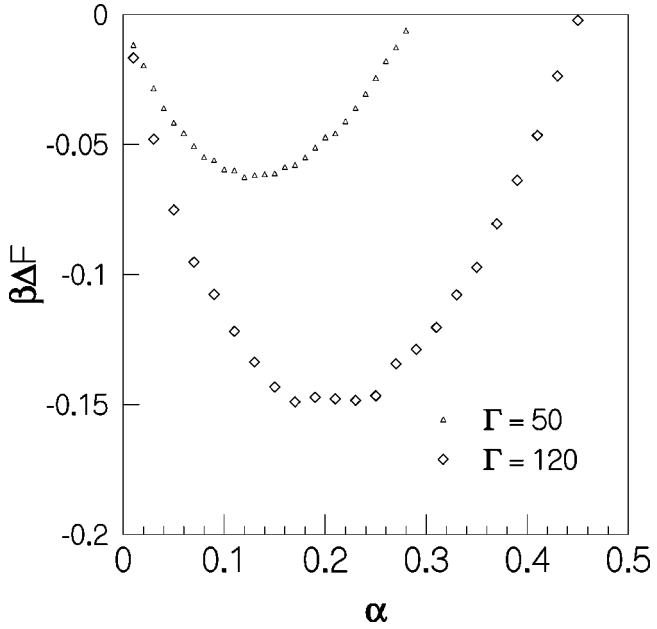

FIG. 4. The free energy difference $\beta\Delta F = \beta[F(\alpha) - F(\alpha = 0)]$ of a pair of pinned vortices separated by distance $d = 1.9a_0$ (which corresponds to the nearest-neighbor distance in a triangular lattice) as a function of the amplitude α of angular modulations [see Eq. (4)] for two values of Γ.

eters a_1, b_1, a_2 and b_2 were kept fixed at their optimal values obtained from the calculation with $\alpha = 0$. The free energy was then minimized as a function of the ''mixing'' parameter α and the two angles, θ_1 and θ_2. We found that at low temperatures, the free energy is minimized for a small but nonzero value of α, indicating that some degree of angular order is indeed preferred. The optimal value of α is relatively large if the spacing d between the defects is close to $1.9a_0$ or $3.3a_0$, the distances corresponding to the nearest-neighbor and next-nearest-neighbor spacings of a triangular lattice. The minimum of the free energy is obtained for $\theta_1 = \theta_2$ for all values of d, and as d is increased from one lattice spacing, the optimal value of these angles switches between 0° and 30°, corresponding to the two possible orientations of one of the shortest reciprocal lattice vectors with respect to the line joining two neighboring sites in a triangular lattice. An angle of 30° corresponds to the two pinned vortices being nearest neighbors, and $\theta_1 = \theta_2 = 0°$ to next-nearest neighbors on a triangular lattice.

We then carried out a more accurate variational calculation for $d = 1.9a_0$ (the nearest-neighbor distance in a triangular lattice) in which the values of θ_1 and θ_2 were fixed at 30° and the free energy was minimized with respect to the parameters a_1, b_1, a_2, and b_2 for each value of the mixing parameter α. The results of this calculation for two values of Γ are shown in Fig. 4. It is clear that a small but nonzero value of α is preferred and that this value increases as the temperature is reduced. Similar results were obtained for $d = 3.5a_0$ and $\theta_1 = \theta_2 = 0°$. The optimal values of α for other ''incommensurate'' values of d were found to be substantially smaller.

The results described above show that the unpinned vortices mediate a short-range effective interaction between two pinned vortices. This effective interaction clearly originates from the density modulations induced around a given pinned vortex. An oscillating coupling results, the period of which is determined by a_0, the intrinsic length scale in the homogeneous liquid. This effective interaction involves both radial (translational) and angular (orientational) degrees of freedom. The fact that the effective interaction is short range while the bare intervortex interaction is long range (logarithmic) is a consequence of the screening produced by the unpinned vortices, which can adjust their positions in response to the forces produced by the pinned vortices. It is interesting to note the analogy of this effective interaction with the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between localized electron spins on dilute magnetic impurities in metals, which arises from matching the induced polarizations of the Fermi liquid of conduction electrons with an intrinsic length scale equal to the Fermi length. However, in the case considered here, the effective interaction between the angular (orientational) degrees of freedom is more complicated than in the RKKY case since certain specific orientations defined with respect to the axis joining the two pinned vortices are preferred. In a periodic pin array, this can effectively lead to a crystalline orientation, but for a random array frustration will occur.

The results of our calculation (Fig. 4) show that, if $B > B_\phi$, pinned vortices do not induce a substantial amount of sixfold angular order in their vicinity, even at the lowest temperature considered here. This result is consistent with decoration experiments[14–16] showing that the correlation length associated with sixfold bond-orientational order is very small (about one lattice spacing) when the number of pinning sites is small compared to the number of vortices. However, the interaction described above may play an important role in the freezing transition. If $B > B_\phi$, crystallization of small domains around pinned vortices should dramatically enhance angular correlations and increase the size

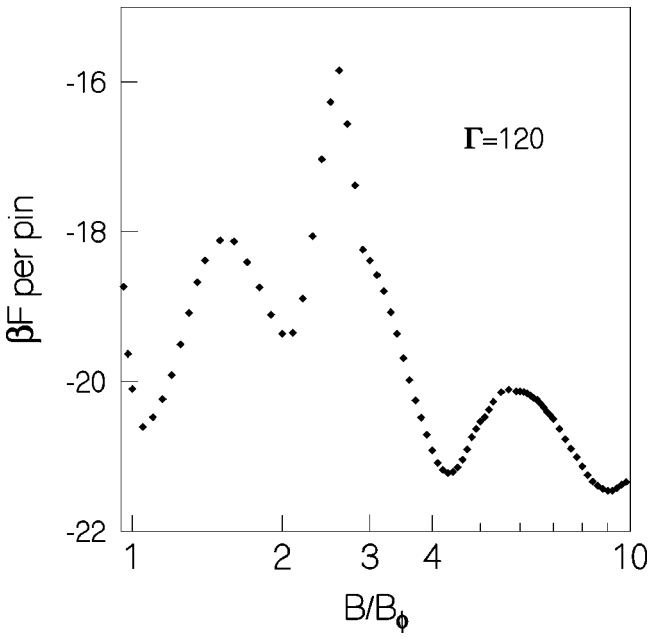

FIG. 5. The pinning part of the free energy per unit cell of a square array of pinning centers as a function of B/B_ϕ where B is the magnetic induction and B_ϕ is the ''matching field.''

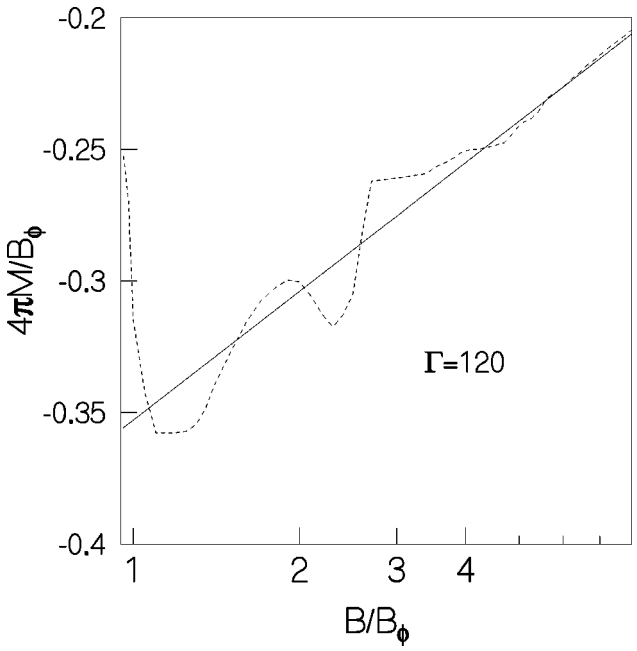

FIG. 6. The magnetization M as a function of the magnetic induction B for a square pin array (dotted line) and for no pinning (solid line) at $\Gamma=120$.

of the interaction, which in turn would control the quenching of local orientations into a glassy state. A detailed description of this process is, however, beyond the scope of the present study.

IV. PERIODIC PIN ARRAY

Let us now turn to the interesting case of a periodic array of strong pinning centers, such as the ones recently fabricated in thin films.[7,8] In these experiments, the defects sit at the points $\{\mathbf{R}_i\}$, which form a square lattice. We first consider the case $B>B_\phi$ and calculate the *reversible* vortex liquid magnetization, given as usual by $M=B/(4\pi)-\partial F/\partial B$. The free energy is the sum of the uniform liquid contribution F_l and that due to the density fluctuations induced by pins [Eq. (2)]. In this calculation, we neglect, for simplicity, the possibility of any angular modulation of the density inhomogeneity produced by a single pinned vortex [i.e., we set the parameter α of Eq. (4) equal to zero]. Such angular modulations are expected to slightly enhance the magnetization anomalies described below. We simply superpose exponentially damped density waves at each pin, i.e., we set $\rho(\mathbf{r})=\rho_l+\Sigma_i\rho'(|\mathbf{r}-\mathbf{R}_i|)$ with ρ' given by Eq. (2). Since one expects the contribution of F_l to $M(H)$ to be quite smooth and any anomaly in the M versus H curve to arise from $F-F_l$, we replace F_l by the usual London expression, neglecting the smoothly varying contribution of thermal fluctuations. For a given B (or ρ_l), the free-energy difference is calculated from Eq. (1) and minimized with respect to a_1, b_1, a_2, and b_2 under the constraints mentioned above. Then $M(H)$ is determined by numerically differentiating the free energy with respect to B. The results obtained for $\Gamma=120$ are shown in Fig. 5 in which the pinning contribution to the free energy per unit cell of the pinning array is plotted as a function of B/B_ϕ, and in Fig. 6 which shows the magnetization M as a function of B/B_ϕ.

The data shown in these two figures contain a few points for $B<B_\phi$. The free energy for such values of B were obtained in the following way. Since the number of vortices is smaller than the number of pinning centers and the temperature is substantially lower than the thermal depinning temperature, all the vortices are expected to be pinned for such values of B. The vortex system then looks very much like a crystal with a few vacancies if B is only slightly lower than B_ϕ. We assume that these vacancies are mobile, so that the average density is obtained by averaging over all possible locations of these vacancies. The density distribution in this situation is then given by a set of Gaussian peaks of equal height and width located at the pinning centers. The width of each Gaussian peak is determined, as before, by the range of the pinning potential. The height of the peak is determined from the requirement that the integrated weight under each peak should be equal to B/B_ϕ, the average occupation probability of each pinning center. The free energy of this state is then calculated using Eq. (1).

It is clear from the data shown in Fig. 5 that the pinning contribution to the free energy has well-defined local minima at $B/B_\phi=1$, 2, and 4. These minima obviously arise due to the commensurability effects discussed above. In particular, each minimum corresponds to a situation in which the length of one of the shortest lattice vectors of the square pinning array coincides with the value of d corresponding to one of the minima of the free energy shown in Fig. 3. The minimum at $B=B_\phi$ corresponds to the nearest-neighbor distance of the pin array being equal to $1.9a_0$, the value of d at which the first minimum of the free energy of Fig. 3 occurs. The minima at $B/B_\phi=2$ and 4 correspond, respectively, to the next-nearest-neighbor and nearest-neighbor distances of the pinning array coinciding with the value of d at the second minimum of the free energy of Fig. 3. We can define an effective pairwise interaction between pinned vortices from

the data of Fig. 3 by subtracting from the free energy its asymptotic value for $d \to \infty$. A sum of this effective interaction over all pairs of sites of the pinning array yields results which are qualitatively similar to the ones shown in Fig. 5. In contrast, a sum of the effective interaction over the pairs of sites of a *random* array of pins shows a smooth variation with B/B_ϕ without the local minima at $B/B_\phi = 2$ and 4, indicating that the broad distribution of the pair separation in a random array washes out the commensurability effects found for a periodic array of pins. This is in agreement with the experimental observation[4–6] of no anomaly in the M versus H curve for $B > B_\phi$ in samples with a random distribution of the pinning centers. The free energy shown in Fig. 5 exhibits a deep local minimum at $B = 4B_\phi$. This is probably due to the fact that the ground state of the vortex system for this value of B is, as found in recent Lorentz microscopy experiments,[8] very close to a triangular lattice, which is the preferred structure of the vortex system in the absence of pinning. We have verified that our ansatz for the density distribution in an unit cell of the pinning array is consistent with the results reported in Ref. 8. In particular, the positions of the peaks of the optimal density distribution found in our calculation are in rough correspondence with the locations of the vortices found in Ref. 8 for the same value of B/B_ϕ.

It is clear from Fig. 6 that in addition to the usual (London) logarithmic behavior, the $M(B)$ curve displays oscillations. These oscillations are clearly correlated with the structure of the free energy shown in Fig. 5. In particular, each anomaly in the $M(B)$ curve is correlated with a local minimum of the free energy. A strong anomaly with a large negative slope occurs near the matching field B_ϕ. At higher fields, weaker but still noticeable anomalies occur near the second and fourth harmonics of the matching field. The anomaly at the second harmonic still displays a negative slope, while around the fourth harmonic the magnetization curve simply flattens. A similar feature has been observed above the irreversibility field but close to B_ϕ in randomly irradiated Tl- and Bi-based cuprates B_ϕ,[4–6] and also in irreversible magnetization measurements for a periodic pin array.[7] All these features have the same origin, namely, the commensurability of the vortex system with the periodic pin array. This leads to a tendency to pin the vortex density (equivalently, the value of B) at values corresponding to the local minima of the free energy occuring at $B = nB_\phi$, $n = 1$, 2, and 4. The strongest possible anomaly happens when the difference $H - nB_\phi$ is perfectly screened, leading to a *plateau* in B, and a local slope of $-1/4\pi$ for the the $M(H)$ curve. Figure 6 shows that the anomalies are weaker in the liquid due to the thermal motion of the unpinned vortices which tend to screen out the commensurability interaction. Nevertheless, the motion of the unpinned vortices remains correlated with the positions of the pinned ones. This is illustrated in Fig. 7 which shows the variation of the density along the diagonal of a square unit cell of the pin lattice for $B/B_\phi = 2.0$ and 1.5. Besides the correlation holes of pinned vortices, the additional feature in the middle reveals a weak pinning potential trapping vortices at the *interstitial* site. Weak pinning of vortices at interstitial sites for $B = 2B_\phi$ has been observed[7] in experiments on superconducting films with a square array of submicron holes. Also, recent Lorentz microscopy experiments[8] have clearly shown the localization

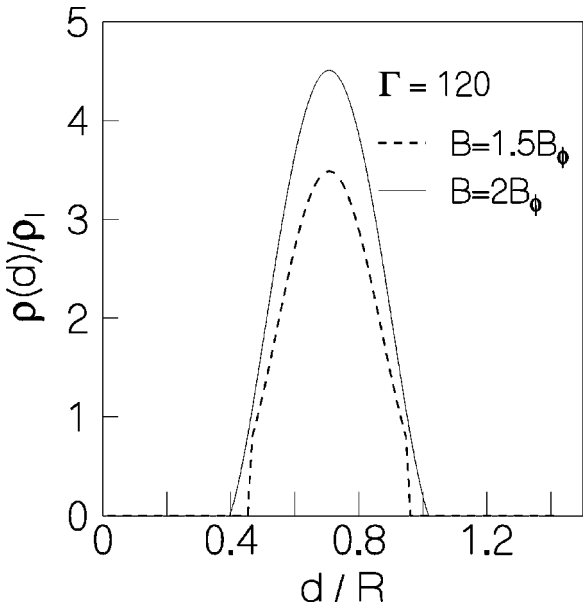

FIG. 7. The vortex density ρ, normalized by the average density ρ_l, along the diagonal of a unit cell of a square pin array for two values of the ratio B/B_ϕ. The distance d is measured from one corner of the unit cell, and R is the lattice constant of the pin array.

of a vortex at the center of each unit cell of the pinning lattice for $B = 2B_\phi$ in a superconducting film with a square array of pinning centers. One notices that this corresponds to the formation of a square vortex lattice with two sublattices, one of vortices strongly pinned at the pinning centers, and the other of vortices weakly pinned at the interstitial sites. It would be interesting to study whether the interstitial vortices exhibit any freezing transition as the temperature is lowered.

V. SUMMARY AND DISCUSSIONS

In summary, we have applied the density-functional theory to vortex liquids with strong disorder. The main result is the short-range and oscillatory coupling between strongly pinned vortices mediated by the moving ones. Weak but possibly relevant orientational effects have been found, and a calculation of magnetization anomalies in a vortex liquid in the presence of a periodic pin array is presented here for the first time. We predict the occurrence of magnetization anomalies at some of the harmonics of the matching field. It would be interesting to look for these anomalies in experiments on samples with a periodic array of pinning centers. We have also studied the structure and the thermodynamics of the vortex liquid at fields close to the matching field. The strong magnetization anomaly found near $B = B_\phi$ may be understood as a precursor of the so-called ''Mott Insulator'' state in the vortex solid.[24]

In this work, we have concentrated on the behavior for $B \geq B_\phi$ because it is difficult to explore the regime $B < B_\phi$ with the present method. Indeed, due to the absence of moving vortices, screening typical of the liquid state would disappear in this case, and the effective interaction between pinned vortices would be close to the bare logarithmic one. Also, since all pins would not be occupied, one must face the

difficult task of locating and averaging over many metastable configurations.[23]

While the calculations described here were carried out for a 2D system, it would not be difficult to extend the method to deal with a layered system with straight columnar defects perpendicular to the layers in an external magnetic field that is also perpendicular to the layers. In this case, the *average* density as a function of the 2D coordinate $\mathbf{r}$ that describes the position on a superconducting layer is expected to be *same* for all layers. The variational forms of Eqs. (2) and (4) would then apply to this situation also. The free energy would be given by a form that is identical to Eq. (1) with the 2D direct pair-correlation function $c(|\mathbf{r}-\mathbf{r}'|)$ replaced by $\Sigma_n c(nd,|\mathbf{r}-\mathbf{r}')$, where n is an integer that denotes the separation between two layers. Since the direct correlation function falls off rapidly with increasing n[19] in strongly anisotropic materials such as BSCCO, the results obtained from such a calculation would be similar to the ones reported here. The interlayer correlations are, in fact, expected to enhance the effects found in the present work.

A remark should be added in this context. Previous calculations[18,19] of the melting of the flux lattice in clean layered superconductors using the same density functional as the one used here reproduce the correct location and slope of the melting line in the B-T plane, but predict the wrong sign for the density discontinuity at the first-order melting transition. This discrepancy is numerically small in magnitude—the calculations predict a small decrease of the density of the vortex solid at melting, whereas experiments[25] show a very small increase. However, this discrepancy is significant in that it amounts to a violation of the Clausius-Clapeyron equation of thermodynamics. The reason for this discrepancy is not completely clear. The peculiar ''icelike'' volume change at the flux lattice melting transition is believed[26] to be due to the line character of vortices, together with their long-range interactions. This suggests that the most probable cause of the discrepancy in the calculations of Refs. 18 and 19 is the approximation made there in the treatment of interlayer density correlations. Problems arising from an approximate treatment of interlayer correlations are, of course, not present in the two-dimensional (one layer) calculations described in the present paper. They should not be too serious in the 3D generalization either since we only address properties inside the liquid phase, not the flux lattice melting transition.

An approximate analytic calculation of the thermodynamic properties of a strongly pinned vortex liquid was carried out recently by Bulaevskii, Vinokur, and Maley.[10] We believe that our work improves upon the treatment of this paper by taking into account the correlations present in the vortex liquid through the term in the density functional that involves the direct correlation function $c(r)$ {the entropic effects considered in Ref. 10 are described by the first term of the density functional [Eq. (1)] used in our study}. In particular, the commensurability effects we have found, originating from the short-range correlations present in the vortex liquid, would not be accessible in the calculation described in Ref. 10. Our results agree qualitatively with those of Ref. 10 where they overlap.

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